

Heat transfer in rapidly solidifying supercooled pure melt during final transient

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Abstract

The heat transfer model for a one-dimensional supercooled melt during the final stage of solidification is considered. The Stefan problem for the determination of the temperature distribution is solved under the condition that (i) the interface approaches the specimen surface with a constant velocity V ; (ii) the latent heat of solidification linearly depends on the interface temperature; (iii) all the physical quantities given at the phase boundary are presented by linear combinations of the exponential functions of the interface position. First we find the solution of the corresponding hyperbolic Stefan problem within the framework of which the heat transfer is described by the telegraph equation. The solution of the initial parabolic Stefan problem is then found as a result of the limiting transition $V/V_H \rightarrow 0$ ($V_H \rightarrow \infty$), where V_H is the velocity of the propagation of the heat disturbances, in which the hyperbolic heat model tends to the parabolic one.

Keywords: Solidification, Final transient, Heat transfer, Stefan problem, Telegraph equation

1. Introduction

The process of rapid solidification is a well established method for the production of metastable solid states of different nature making it possible to study new mechanisms of crystal growth and produce materials with radically new physical properties [1].

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In rapid solidification experiments very high velocities of phase interface can be reached. Such conditions occur during solidification of the undercooled melts or recrystallization after pulsed-laser irradiation of a solid surface. When the interface velocity reaches some critical value diffusion-temperature field in the bulk of both phases can significantly deviate from local equilibrium [2, 3]. In this case both the diffusion and heat fluxes are no longer defined by the classical Fick's and Fourier's laws relating the diffusion and heat fluxes correspondingly to the gradients of a solute concentration and temperature. The simplest generation of Fick's and Fourier's laws taking into account the relaxation to local equilibrium in the diffusion and the heat field is given by the Maxwell-Cattaneo model and leads to the hyperbolic transport equations [8].

In the past two decades a great body of studies, devoted to the local nonequilibrium heat and mass transport during rapid solidification, has been executed [2, 3, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. The numerical estimates show that under conditions of experimentally achievable interface velocities local equilibrium is only disturbed in the diffusion field, while the heat field can be described in the local-equilibrium approximation within the scope of the conventional parabolic heat conduction model [2, 3]

The currently existing analytical models of the directional solidification processes usually consider the initial transient and the motion of the planar front far from the boundaries of a system [19, 20, 21]. The investigation of the final transient is practically absent. Meanwhile, besides a purely academic problem there exists considerable practical interest as well because the final study of solidification process influences the formation of the surface layer of the materials, their surface physical-chemical characteristics and the distributions of different defects [22, 23, 24].

The final transient of a binary melt solidification has been analytically considered by Smith et. al. in the work [25] (also see [26], p.278). In the local equilibrium approximation the authors have calculated the terminal solute distribution of a formed solid. However the found distribution has divergence at the surface of the specimen that may be caused, among other reasons, by neglect of the temperature changes during the interface motion near the surface. Because of the thermodynamic relationship between the interface temperature and the solute concentration, resulting from the phase diagram, such changes can lead to further solute redistribution in the bulk of the specimen. In this connection it is of interest to initially investigate the evolution of the temperature field of the solidifying pure melt during the

final transient.

In general, the problem of the determination of the temperature field during solidification of a melt is known as the Stefan problem. It consists in solving of the heat conduction equation for a temperature T of each phase with the boundary conditions at the moving interface and in the one-dimensional form is written as

$$\rho c_p \frac{\partial T_{L,S}}{\partial t} = \lambda \frac{\partial^2 T_{L,S}}{\partial x^2}, \quad (1)$$

$$T_L = T_S, \quad (2)$$

$$q_L - q_S = QV, \quad (3)$$

where indexes L and S are respectively related to the liquid and the solid phase, ρ is the density, c_p is the specific heat and λ is the thermal conductivity (for simplicity, all material characteristics are assumed to be constant and identical within the phases and at the interface). Equation (2) represents the condition of the continuity of the temperature across the interface and equation (3) defines the condition of a heat balance at the interface, where $q_{L,S} = -\lambda \partial T_{L,S} / \partial x$ is the heat flux, Q is the latent heat of solidification and V is the velocity of the interface. In addition, at the surface of the specimen the boundary conditions must be given.

From the thermodynamic point of view the velocity V is determined by the undercooling of the interface $\Delta T = T_m - T_i$, where T_m is the equilibrium temperature of solidification and T_i is the interface temperature, $V = f(\Delta T)$, so that at $\Delta T = 0$, $V = f(0) = 0$. For so-called normal crystal growth it is assumed that

$$V = \mu \Delta T \quad (4)$$

where μ is the kinetic coefficient characterizing atomic attachment kinetics at the interface [19]. When the undercooling of the interface ΔT is large enough, the relationship (4) can no longer hold. This takes place when the melt is initially supercooled. In a number of experiments with pure metals, as well as by means of molecular-dynamic simulation [27, 28, 29, 30] it has been shown that at the beginning the growth velocity increases with increasing undercooling ΔT reaching a maximum value and then above some critical undercooling ΔT^* , V is practically kept constant in some region ΔT (also see [19], p.18). In what follows we shall presume that the function $V = f(\Delta T)$ has such properties.

When the undercooling is large enough the amount of latent heat released on the solidification front may prove to be deficient to heat the interface to the temperature T_m . In this case the undercooling at the interface will be different from zero during the whole solidification process, $\Delta T \neq 0$, and the solid phase will reach the surface of the specimen with a finite velocity, $V_f = f(\Delta T_f) \neq 0$. When the interface moves in the near surface region the undercooling ΔT , generally speaking, will change, at the same time also changing the growth velocity V . However, assuming that V_f is high enough, due to high undercooling [1], and ΔT changes within the region for which velocity V depends slightly on ΔT , one can consider that the interface moves near the surface with approximately constant velocity V equal to V_f . It should be noted that there exists a substantial distinction from the situation in the initial transient when the interface velocity changes from zero to a steady state value.

The behavior of the temperature T_i , the heat fluxes $q_{L,S}$ and the latent heat Q at the moving interface essentially affects the evolution of the thermal field in the bulk of the phases. Giving different models of their behavior at the interface, one can consider various models of the solidification process. In the present study we consider the exactly solvable model of solidification within the scope of which any physical quantity F (the temperature, the heat flux, etc.) is given at the interface as

$$F(x, t)|_{t=t(x)} = A_0^{(F)} + A_1^{(F)} e^{-\gamma_1 x/2} + A_2^{(F)} e^{-\gamma_2 x/2} \dots, \quad (5)$$

where $t = t(x)$ determines the path of the interface position and the coefficients $A_n^{(F)}$ and the powers of the exponents γ_n must be defined from the phase boundary conditions and the boundary condition at the surface of the system. It is worth noting that an expression of similarly type has been obtained for the solute distribution in the work [25].

As regards the latent heat of the solidification it is normally assumed to be constant and is empirically defined for the equilibrium temperature T_m as $Q = Q_m = kT_m$ ($k = \text{const}$) ([31], p.185). If the undercooling of the interface is high enough, it is reasonable to define the variable latent heat as $Q = kT_i = Q_m - k\Delta T$ that will be used in what follows.

Thus for the determination of the temperature field within the scope of the given model we seek the solution of the one-dimensional heat conduction equation (1) with the boundary conditions (2), (3) and (5) when the interface approaches to the surface with a constant velocity V and the latent heat linearly depends on the undercooling ΔT .

As has been noted above, the temperature field in a rapid solidifying melt can be considered within the scope of the parabolic model (1)-(3). However to obtain the solution of interest we shall initially consider an auxiliary problem, namely, the corresponding Stefan problem for the hyperbolic heat conduction equation (see, for example, [5, 12]). It turns out that the boundary conditions given at the moving interface are more simply taken into account within the scope of the hyperbolic model. As is known, the hyperbolic model of heat conduction, based on the telegraph equation, gives the finite velocity of the propagation of the heat disturbances in matter V_H and is reduced to the parabolic model (1) in the limit $V_H \rightarrow \infty$ [8]. The idea of the work is that initially the solution of the hyperbolic Stefan problem with arbitrary ratio of the velocities $V/V_H < 1$ is solved and then the limiting transient, $V/V_H \rightarrow 0$, to the solution of the parabolic problem is executed.

The work is organized as follows. In Sec.2 the hyperbolic Stefan problem corresponding to the boundary problem (1)-(3), (5) is considered. The solution of the telegraph equation is found by the Riemann method within the scope of which the boundary conditions given at arbitrary moving boundary are automatically taken into account. On the basis of this solution the heat fluxes and the temperature fields both in the liquid phase and in the near interface region of the solid are determined. The subsequent limiting transition $V/V_H \rightarrow 0$ and the solution of the parabolic problem are given in Sec.3. The conclusion is presented in Sec.4. The Riemann method and its application to the presented problem are contained in the Appendices.

2. Hyperbolic model

The hyperbolic model of the heat conduction starts from the Maxwell-Cattaneo relaxation equation for the heat flux [8]. In the one-dimensional form this equation for the liquid phase is

$$q_L + \tau \frac{\partial q_L}{\partial t} = -\lambda \frac{\partial T_L}{\partial x}, \quad (6)$$

where $\tau = a/V_H^2$ is the time of the relaxation of the heat flux to its local equilibrium value defined by the Fourier's law and $a = \lambda/\rho c_p$ is the thermal diffusivity.

Equation (6) in combination with the conservation law

$$\rho c_p \frac{\partial T_L}{\partial t} = -\frac{\partial q_L}{\partial x}, \quad (7)$$

gives rise to the hyperbolic transport equations

$$\tau \frac{\partial^2 T_L}{\partial t^2} + \frac{\partial T_L}{\partial t} = a \frac{\partial^2 T_L}{\partial x^2} \quad (8)$$

$$\tau \frac{\partial^2 q_L}{\partial t^2} + \frac{\partial q_L}{\partial t} = a \frac{\partial^2 q_L}{\partial x^2}. \quad (9)$$

The equation of the type (8) or (9) is known as the telegraph equation. At $\tau \rightarrow 0$ (or $V_H \rightarrow \infty$) the equations (8) and (9) are reduced to the parabolic heat conduction equation (1).

Now let us consider the supercooled pure melt initially occupying the half-space $x \geq 0$. The planar front of solidification forms in the infinitely removed region at $t = -\infty$ and moves in parallel to the specimen surface fixed at $x = 0$. As it has been noted in the Introduction when the undercooling is large enough the interface will move in the near surface region with the approximately constant velocity $V = V_f$ along the path $x + Vt = 0$. In this case the region occupied by the melt in the final stage of the solidification process is given by the inequality $0 \leq x \leq -Vt$ ($t \leq 0$). Therefore in the plane (x, t) the liquid phase occupies the region $x + Vt \leq 0, x \geq 0, t \leq 0$. At the interface the condition of the heat balance (3) holds

$$(q_L - q_S)|_{x+Vt=0} = -VQ|_{x+Vt=0}, \quad (10)$$

Now we consider the heat flux q_L in more detail. Introducing dimensionless variables t/τ , $x/\tau V_H$ in the equation (9), one obtains

$$\frac{\partial^2 \tilde{q}_L}{\partial t^2} + \frac{\partial \tilde{q}_L}{\partial t} = \frac{\partial^2 \tilde{q}_L}{\partial x^2}, \quad (11)$$

where the former notations (x, t) have been used for new variables, $\tilde{q}_L = q_L/(Q_m V_H)$ is a dimensionless heat flux. The boundary condition (10) in the dimensionless form is written as

$$(\tilde{q}_L - \tilde{q}_S)|_{x+\alpha t=0} = -\alpha \tilde{Q}|_{x+\alpha t=0}, \quad (12)$$

where $\tilde{q}_S = q_S/(Q_m V_H)$, $\tilde{Q} = Q/Q_m$ and $\alpha = V/V_H$ is the dimensionless parameter. In addition, we assume that at the surface the equality should be fulfilled

$$\tilde{q}_L(xt)|_{x=0} = 0 \quad (t \leq 0), \quad (13)$$

expressing the condition of the absence of the heat flux through the surface. Finally, the solution of (11) is sought in the near surface region at $X \equiv$

$x + \alpha t \leq 0$, $x \geq 0$, $t \leq 0$ occupied by the liquid phase while the solid occupies the region $X \geq 0$ (see fig. A.1b in Appendix).

Now we consider the case of $\alpha < 1$. Suppose that at the moving interface residing in an arbitrary point x near the surface at the moment $t = -x/\alpha$ the flux \tilde{q}_L and its time derivative $\partial\tilde{q}_L/\partial t$ are known

$$\tilde{q}_L(xt)|_{t=-x/\alpha} = q_0(x) \quad \frac{\partial\tilde{q}_L(xt)}{\partial t}|_{t=-x/\alpha} = q_1(x), \quad (14)$$

where the functions $q_0(x)$ and $q_1(x)$ will be specified further.

If the functions $q_0(x)$ and $q_1(x)$ are known the solution of the equation (11) satisfying the conditions (14) in the region $X \leq 0$ at $\alpha < 1$ can be found by the Riemann method [32] (for details see Appendix A) and has the form

$$\begin{aligned} \tilde{q}_L(xt) = & \frac{1}{2} \left\{ \varphi\left(-\alpha \frac{x+t}{1-\alpha}\right) \exp\left[\frac{X}{2(1-\alpha)}\right] + \varphi\left(\alpha \frac{x-t}{1+\alpha}\right) \exp\left[-\frac{X}{2(1+\alpha)}\right] \right\} \\ & - \frac{1}{2} e^{-t/2} \int_{-\frac{\alpha(x+t)}{1-\alpha}}^{\frac{\alpha(x-t)}{1+\alpha}} dx_1 \psi(x_1) e^{-x_1/2\alpha} J_0\left(\frac{1}{2} \sqrt{(x-x_1)^2 - (t+x_1/\alpha)^2}\right) \\ & + \frac{X}{4\alpha} e^{-t/2} \int_{-\frac{\alpha(x+t)}{1-\alpha}}^{\frac{\alpha(x-t)}{1+\alpha}} dx_1 \varphi(x_1) e^{-x_1/2\alpha} \frac{J'_0\left(\frac{1}{2} \sqrt{(x-x_1)^2 - (t+x_1/\alpha)^2}\right)}{\sqrt{(x-x_1)^2 - (t+x_1/\alpha)^2}}, \end{aligned} \quad (15)$$

where

$$\varphi(x) = q_0(x), \quad \psi(x) = \frac{1}{2} q_0(x) - \frac{1}{\alpha} q'_0(x) - \frac{1-\alpha^2}{\alpha^2} q_1(x) \quad (16)$$

and $J_0(x)$ is the Bessel function of zero order.

In accordance with what was said in the Introduction all the quantities given at the phase interface are represented by linear combinations of the exponential functions (5). In particular, let $\varphi(x)$ and $\psi(x)$ be given by the expansions

$$\varphi(x) = A_0 + A_1 e^{-\gamma_1 x/2} + A_2 e^{-\gamma_2 x/2} \dots, \quad (17)$$

$$\psi(x) = B_0 + B_1 e^{-\gamma_1 x/2} + B_2 e^{-\gamma_2 x/2} \dots, \quad (18)$$

where constants $\gamma_n \geq 0$, A_n and B_n will be specified in what follows. After the substitution of (17) and (18) in (15) and the calculation of the integrals (details in Appendix B), we obtain

$$\tilde{q}(xt) = \sum_{n \geq 0} e^{-\gamma_n x/2} \left\{ A_n^{(-)} \exp \left[\frac{\gamma_n^{(+)} X}{2(1-\alpha^2)} \right] + A_n^{(+)} \exp \left[\frac{\gamma_n^{(-)} X}{2(1-\alpha^2)} \right] \right\}, \quad (19)$$

where the following notations have been introduced

$$\gamma_n^{(\pm)} = \gamma_n + \alpha \pm \sqrt{\alpha^2 \gamma_n^2 + 2\alpha \gamma_n + \alpha^2} \geq 0; \quad (20)$$

$$A_n^{(\pm)} = \frac{A_n}{2} \pm B_n \frac{\delta_n}{\nu_n}; \quad (21)$$

$$\delta_n = \frac{\alpha}{1 + \alpha \gamma_n}; \quad \nu_n = \sqrt{1 - \frac{\delta_n^2}{\alpha^2} (1 - \alpha^2)}. \quad (22)$$

Let us determine the parameters γ_n , A_n and B_n in such a way as to satisfy the balance condition (12) and the boundary condition at the sample surface (13).

2.1. The determination of the parameters

Now consider the boundary condition (13). Taking into account that $\gamma_0 = 0$, $\delta_0 = \alpha$, $\nu_0 = \alpha$, $\gamma_0^{(\pm)} = \alpha \pm \alpha$ and using the equation (19), we have for arbitrary small $t < 0$

$$\begin{aligned} \tilde{q}(x, t)|_{x=0} &= A_0^{(-)} \exp \frac{2\alpha^2 t}{2(1-\alpha^2)} + A_0^{(+)} + \\ &+ A_1^{(-)} \exp \frac{\gamma_1^{(+)} \alpha t}{2(1-\alpha^2)} + A_1^{(+)} \exp \frac{\gamma_1^{(-)} \alpha t}{2(1-\alpha^2)} + \\ &+ A_2^{(-)} \exp \frac{\gamma_2^{(+)} \alpha t}{2(1-\alpha^2)} + A_2^{(+)} \exp \frac{\gamma_2^{(-)} \alpha t}{2(1-\alpha^2)} + \dots = 0. \end{aligned} \quad (23)$$

If all the powers of the exponentials are different then $\tilde{q}(0, t) = 0$ can be only at $A_n = B_n = 0$. However if each exponential function appears in the equation (23) at least twice then this can lead to nonzero A_n and B_n . Bearing in mind this circumstance we determine γ_n so that the following equalities hold

$$\gamma_n^{(-)} = \gamma_{n-1}^{(+)} \quad n = 1, 2, 3, \dots, \quad (24)$$

Table 1: The parameters of the equation (19)

n	0	1	2	3	4
γ_n	0	$\frac{4\alpha}{1-\alpha^2}$	$\frac{4\alpha(3+\alpha^2)}{(1-\alpha^2)^2}$	$\frac{8\alpha(3+\alpha^2)(1+\alpha^2)}{(1-\alpha^2)^3}$	$\frac{8\alpha(1+\alpha^2)(\alpha^4+10\alpha^2+5)}{(1-\alpha^2)^4}$
$\gamma_n^{(+)}$	2α	$\frac{8\alpha}{1-\alpha^2}$	$\frac{2\alpha(3+\alpha^2)^2}{(1-\alpha^2)^2}$	$\frac{32\alpha(1+\alpha^2)^2}{(1-\alpha^2)^3}$	$\frac{2\alpha(\alpha^4+10\alpha^2+5)^2}{(1-\alpha^2)^4}$
$\gamma_n^{(-)}$	0	2α	$\frac{8\alpha}{1-\alpha^2}$	$\frac{2\alpha(3+\alpha^2)^2}{(1-\alpha^2)^2}$	$\frac{32\alpha(1+\alpha^2)^2}{(1-\alpha^2)^3}$

in which $\gamma_{n-1}^{(+)}$ (and respectively γ_{n-1}) are considered to be known ¹. Taking into account the notation (20) and resolving the equation (24) in relation to γ_n , one obtains

$$(1 - \alpha^2)(\gamma_n)_{12} = \gamma_{n-1}^{(+)} \pm \sqrt{\alpha\gamma_{n-1}^{(+)}[2(1 - \alpha^2) + \alpha\gamma_{n-1}^{(+)}]}. \quad (25)$$

At $n = 1$ and $\gamma_0^{(+)} = 2\alpha$ the equation (25) gives

$$\gamma_1 = \frac{4\alpha}{1 - \alpha^2}.$$

The second value $\gamma_1 = 0$ is the extraneous root of the equation (24) at $n = 1$. After the determination of γ_1 the values $\gamma_1^{(\pm)}$ appearing in (19) can be found from the equation (20). Along a similar line one can obtain the values γ_n , $\gamma_n^{(\pm)}$ for $n > 1$. In Table 1 these values are given for $n \leq 4$. As is seen from the table $\gamma_n \sim (1 - \alpha^2)^{-n}$, $\gamma_n^{(+)} \sim (1 - \alpha^2)^{-n}$, $\gamma_n^{(-)} \sim (1 - \alpha^2)^{-n+1}$. The case of an arbitrary n is easily proved by induction using (25).

Under condition (24), the equation (23) holds, if

$$\begin{aligned} A_0^{(+)} &= A_0/2 + B_0 = 0 \\ A_0^{(-)} &= A_0/2 - B_0 = A_0 \\ A_n^{(+)} &= -A_{n-1}^{(-)} \quad (n \geq 1) \end{aligned} \quad (26)$$

Finally taking into account the equalities (26), the expression (19) can be rewritten in the form

$$\tilde{q}(xt) = \sum_{n \geq 0} A_{n+1}^{(+)} (e^{-\gamma_{n+1}x/2} - e^{-\gamma_n x/2}) \exp \left[\frac{\gamma_{n+1}^{(-)} X}{2(1 - \alpha^2)} \right]. \quad (27)$$

¹The equation $\gamma_n^{(+)} = \gamma_{n-1}^{(+)}$ either has no the solutions or does not give the new ones.

2.2. The temperature field

The temperature field in the liquid phase can be found in the same way as the heat flux has been defined. The resulting expression for the dimensionless temperature \tilde{T}_L takes the form

$$\tilde{T}_L(xt) = a_0^{(+)} + \sum_{n \geq 0} \{a_n^{(-)} e^{-\gamma_n x/2} + a_{n+1}^{(+)} e^{-\gamma_{n+1} x/2}\} \exp\left[\frac{\gamma_{n+1}^{(-)} X}{2(1 - \alpha^2)}\right], \quad (28)$$

where $\tilde{T}_L = \rho c_p (T_L - T_m)/Q_m$. The constants $a_n^{(\pm)}$ can be expressed in terms of the parameters determining T and $\partial T/\partial t$ at the interface by the equations of the type (16)-(18) and (21).

Substituting the expressions for the flux (27) and the temperature (28) into the energy consideration law (7) and equating the coefficients at the linear independent functions, one can express the constants $a_n^{(\pm)}$ in terms of $A_n^{(+)}$ appearing in (27). The corresponding expressions will be given for the case of the parabolic model.

2.3. The solid phase

The heat flux q_S and the temperature T_S in the solid satisfy the equations

$$\frac{\partial^2 \tilde{q}_S}{\partial t^2} + \frac{\partial \tilde{q}_S}{\partial t} = \frac{\partial^2 \tilde{q}_S}{\partial x^2}; \quad \frac{\partial^2 \tilde{T}_S}{\partial t^2} + \frac{\partial \tilde{T}_S}{\partial t} = \frac{\partial^2 \tilde{T}_S}{\partial x^2} \quad (29)$$

where $\tilde{q}_S = q_S/(Q_m V_H)$, $\tilde{T}_S = \rho c_p (T_S - T_m)/Q_m$.

For the complete determination of the temperature field in the liquid the interface boundary conditions (2) and (12) depending on the solid temperature and the heat flux must be used. For their determination it will suffice to consider the solutions of the equations (29) in the region near the interface defined by the inequalities $X > 0$, $x + t < 0$ (see fig. A.1c). The solutions of the equations (29) in this region can be obtained in the same way as for the liquid phase. The application of the Riemann method in the indicated region gives for the heat flux

$$\tilde{q}_S(xt) = \sum_{n \geq 0} e^{-\gamma_n x/2} \left\{ \tilde{A}_n^{(-)} \exp\left[\frac{\gamma_n^{(+)} X}{2(1 - \alpha^2)}\right] + \tilde{A}_n^{(+)} \exp\left[\frac{\gamma_n^{(-)} X}{2(1 - \alpha^2)}\right] \right\}, \quad (30)$$

where $\gamma_n^{(\pm)}$ are given by the equality (20) and the constants $\tilde{A}_n^{(\pm)}$ can be expressed in terms of the parameters determining the flux \tilde{q}_S and its time derivative at the interface by the equalities of the type (21).

The expression for the temperature \tilde{T}_S is analogously written down as

$$\tilde{T}_S(xt) = \sum_{n \geq 0} e^{-\gamma_n x/2} \left\{ \tilde{a}_n^{(-)} \exp \left[\frac{\gamma_n^{(+)} X}{2(1-\alpha^2)} \right] + \tilde{a}_n^{(+)} \exp \left[\frac{\gamma_n^{(-)} X}{2(1-\alpha^2)} \right] \right\}. \quad (31)$$

3. The parabolic model

As has been indicated above the transition to the parabolic model is executed by the limit $\alpha = V/V_H \rightarrow 0$ ($V_H \rightarrow \infty$). Using table 1 and the equation (25) it is easy to show by the induction for any n that for small α

$$\begin{aligned} \gamma_n &\simeq 2n(n+1)\alpha & \alpha \rightarrow 0 & \quad (\alpha \neq 0) \\ \gamma_n^{(-)} &\simeq 2n^2\alpha \\ \gamma_n^{(+)} &\simeq 2(n+1)^2\alpha. \end{aligned} \quad (32)$$

When the relationships (32) are fulfilled the expressions for the temperature \tilde{T}_L and the flux \tilde{q}_L in the liquid phase are written down in the form

$$\tilde{T}_L(xt) = a_0^{(+)} + \sum_{n \geq 0} \frac{A_{n+1}^{(+)}}{\alpha(n+1)} \{e^{-\gamma_{n+1}x/2} + e^{-\gamma_n x/2}\} e^{\gamma_{n+1}^{(-)} X/2} \quad (33)$$

$$\tilde{q}_L(xt) = \sum_{n \geq 0} A_{n+1}^{(+)} \{e^{-\gamma_{n+1}x/2} - e^{-\gamma_n x/2}\} e^{\gamma_{n+1}^{(-)} X/2} \quad (34)$$

The constants $a_n^{(\pm)}$ in the equation (28) for \tilde{T}_L have been defined in such a way as to satisfy the conservation law (7) (see the end of section 2.2).

From expression (33) it is seen that the disturbances of the temperature field ahead of the solidification front propagate only over distances in the order of $l \lesssim 2\tau V_H / \gamma_1^{(-)} = a/V$ (in the dimensional variables). Therefore, if the interface is removed from the surface at the distance $l \sim a/V$, the surface still remains at the initial temperature T_0 ². It is supposed, of course, that the constant interface velocity approximation holds over distances in the order of a/V from the surface. At $x = 0$ and $V|t| \sim a/V$ in the expression (33) one can neglect by sum ($|X| = |Vt| \sim a/V$) and write down for the temperature at the surface

$$\tilde{T}_L|_{x=0} = \Delta \approx a_0^{(+)},$$

²For example, for Ni $a = 12 \cdot 10^{-6} m^2/s$, $V \sim 20 m/s$, $a/V \sim 0.6 \mu m$. [28].

where $\Delta = \rho c_p (T_0 - T_m)/Q_m < 0$ is the initial undercooling of the melt.

Now let us consider the temperature field in the solid phase. The equalities (30) and (31) hold in the region between the straight lines $x + \alpha t = 0$ and $x + t = 0$ (see fig. A.1c), or in the dimensional variables, between the straight lines $x + Vt = 0$ and $x + V_H t = 0$. At $V_H \rightarrow \infty$ the second line goes to the straight line $t = 0$, $0 \leq x < \infty$ and the region of interest to us will be given by the inequality $-Vt < x < \infty$, spreading over the whole solid phase.

The variable part of the expressions (30) and (31) in the dimensional coordinates (x, t) is determined by the exponents

$$e^{(n+1)V[x+(n+1)Vt]/a}, \quad e^{-nV[x-nVt]/a} \quad (V/V_H \ll 1).$$

It is easy to see that at small t the terms containing the first exponent (are proportional to $\tilde{A}_n^{(-)}$ or $\tilde{a}_n^{(-)}$) with increasing x will indefinitely increase. In order to avoid such nonphysical behavior we put $\tilde{A}_n^{(-)} = \tilde{a}_n^{(-)} = 0$ and introduce the notations $A_n^{(S)} = \tilde{A}_n^{(+)}$. Turning back to the dimensionless coordinates, let us write down the expressions (30) and (31) at the small α in the form

$$\tilde{T}_S(xt) = a_0^{(S)} + \sum_{n \geq 1} \frac{A_n^{(S)}}{\alpha n} e^{-\gamma_n x/2} e^{\gamma_n^{(-)} X/2} \quad (35)$$

$$\tilde{q}_S(xt) = \sum_{n \geq 1} A_n^{(S)} e^{-\gamma_n x/2} e^{\gamma_n^{(-)} X/2}, \quad (36)$$

where the constants $\tilde{a}_n^{(+)}$ have been determined so that the conservation law (7) is obeyed. It is easy to check that the expressions (33)-(36) satisfy the heat conduction equations

$$\frac{\partial T_{LS}}{\partial t} = \frac{\partial^2 T_{LS}}{\partial x^2}, \quad \frac{\partial q_{LS}}{\partial t} = \frac{\partial^2 q_{LS}}{\partial x^2}$$

and the Fourier's law is fulfilled, $\tilde{q}_{L,S} = -\partial \tilde{T}_{L,S} / \partial x$.

3.1. The temperature field

For the determination parameters appearing in equations (33)-(36) we use the condition of continuity of the temperature across the interface (2). The detailed calculations are given in Appendix C. The final expression for

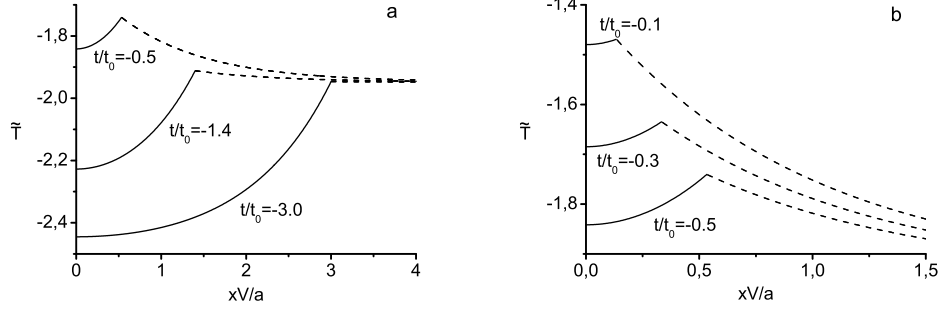


Figure 1: The temperature profiles for different moments of time. The dashed lines correspond to the temperature distribution in the solid phase, the solid lines correspond to the liquid phase; $t_0 = a/V^2$.

the temperature of the liquid phase can be represented in the dimensional coordinates (x, t) as

$$\begin{aligned} \tilde{T}_L(x, t) &= \Delta + \frac{(1 + b\Delta)}{1 - b} \sum_{n \geq 1} C_n \left\{ e^{nV(x+nVt)/a} + e^{-nV(x-nVt)/a} \right\} \quad (37) \\ C_1 &= 1; \quad C_n = b^{n-1} \prod_{k=2}^n \frac{1}{(2k-1-b)} \quad (n \geq 2); \\ (0 \leq x \leq -Vt, \quad t \leq 0); \end{aligned}$$

where $b = T_Q/T_m$ and $T_Q = Q_m/\rho c_p$. For metals the dimensionless parameter b varies through the range $0 < b < 1$. For example, for Ni, $T_m = 1726K$, $T_Q = Q_m/\rho c_p = 397K$ and $b = T_Q/T_m = 0,23$ [10].

Similarly one can write down for the solid phase

$$\begin{aligned} \tilde{T}_S(x, t) &= \frac{1 + \Delta}{1 - b} + \frac{1 + b\Delta}{1 - b} \sum_{n \geq 1} \frac{2n+1}{2n+1-b} C_n e^{-nV(x-nVt)/a}, \quad (38) \\ (-Vt \leq x, \quad t \leq 0). \end{aligned}$$

It is easily seen that each term in the brace (37) represents the superposition of two heat waves propagating in the mutually opposing directions with the velocity nV .

3.2. Numerical results

Figures 1-2 present the temperature profiles obtained from the equations (37), (38) for $\Delta = -2.5$ (supercooling) and $b = 0,23$.

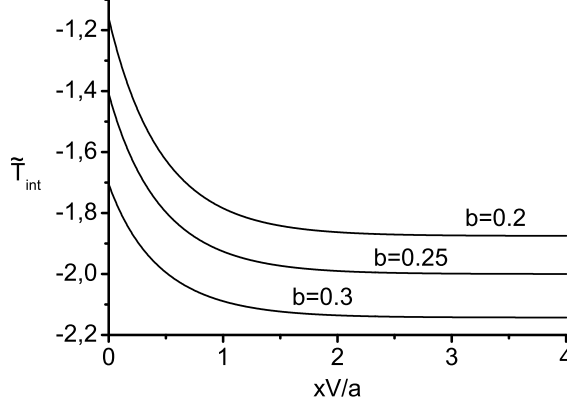


Figure 2: The temperature at the interface depending on the distance to the free surface for different values of the parameter $b = T_Q/T_m$.

The temperature curves for some moments of time are shown in figure 1. The dashed lines are the temperature distributions in the solid phase, the solid lines give the temperature field in the liquid phase. As is seen from figure 1a when the interface is relatively far from the surface ($t/t_0 = -3, t_0 = a/V^2$) the temperature of the solid phase is constant, and the temperature of the liquid phase falls to approximately the initial temperature of the melt T_0 ($\tilde{T}_L|_{x=0} \approx \Delta = (T_0 - T_m)/T_Q = -2.5$) at the surface. When the interface moves close enough to thermal isolated surface (figure 1b), the released latent heat gives rise to the gradual heating of both the liquid phase and the near-interface region of the solid.

In the figure 2 the dependence of the interface temperature on the parameter b is shown. From the figure it is also seen that the interface appears on the surface (at $x = 0$) in the supercooled state, $|T_i - T_m|/T_Q > 1$, providing high final velocity of the solidification processes $V = V_f$.

4. Conclusion

In the given work we have considered a one-dimensional model of the heat conduction in the supercooled melt during the final transient. Three main assumptions underlie the model. Firstly, it is supposed that the interface approaches the system surface with a constant velocity. Some reasons for this assumption are provided by a number of experimental results and molecular-

dynamic simulation [27, 28, 29, 30, 19] showing that when the undercooling of the melt is large enough the interface velocity can slightly depend on the temperature. The second supposition assumes that the latent heat of solidification linearly depends on the interface temperature. Finally, it is supposed that the physical quantities of interest (the temperature, the heat flux, etc.) given at the interface are presented by linear combination of the exponential functions of the form (5), the parameters of which are determined as part of the general solution of the problem.

Within the scope of the model the exact solution of the one-dimensional Stefan problem (1)-(3), (5) defining thermal distribution in the system when the interface moves near the surface has been found. To this end, initially, the corresponding hyperbolic Stefan problem has been considered within the framework of which the heat transfer is described on the basis of the telegraph equation. The telegraph equation for the heat flux and the temperature in both the liquid phase and the near interface region of the solid has been resolved by the Riemann method. Further we have used the fact that in the limit $\alpha = V/V_H \rightarrow 0$ the hyperbolic heat model is reduced to the parabolic one. Taking into account this circumstance and executing the limiting transition $\alpha \rightarrow 0$ in the expressions for the fluxes (27), (30) and the temperature (28), (31) the thermal distribution in the sample during the final stage of solidification has been obtained.

In conclusion it should be noted, that the given approach allow us to consider also other models of the solidification process differing from model (5). It is likely that the interface boundary conditions in the form of the superposition of exponential functions are the only ones for which the exact solution exists. On the other hand the solution for the heat flux (15) is written down for arbitrary boundary conditions (arbitrary φ and ψ) and opens up the possibility of numerical simulation.

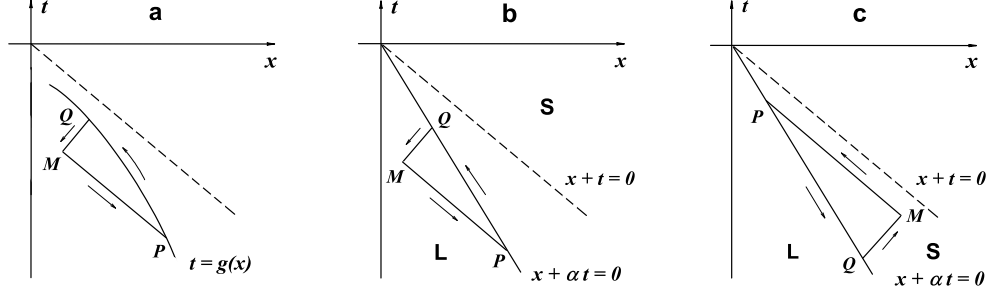


Figure A.1: (a) The figure to the Riemann method. (b) The solution of the equation (11) is sought in the region of the liquid phase $x + \alpha t < 0$. (c) The solutions of the equations (29) are sought in the region of the solid phase situated between straight lines $X = x + \alpha t = 0$ and $x + t = 0$.

Appendix A. The Riemann method

Let it be required to find the solution of the linear hyperbolic equation

$$\frac{\partial^2 \tilde{q}}{\partial t^2} + \frac{\partial \tilde{q}}{\partial t} = \frac{\partial^2 \tilde{q}}{\partial x^2}, \quad (\text{A.1})$$

satisfying the initial conditions given at the curve $\Gamma : t = g(x)$ (see figure A.1a)

$$\begin{aligned} \tilde{q}|_{t=g(x)} &= q_0(x) \\ \frac{\partial \tilde{q}}{\partial t}|_{t=g(x)} &= q_1(x). \end{aligned}$$

The substitution $\tilde{q} = e^{-t/2}u$ makes it possible to lead equation (A.1) to a more simple form

$$\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial t^2} + \frac{1}{4}u = 0, \quad (\text{A.2})$$

with the initial conditions

$$u|_{t=g(x)} = q_0(x)e^{g(x)/2} \equiv \varphi_1(x) \quad (\text{A.3})$$

$$\frac{\partial u}{\partial t}|_{t=g(x)} = (\tfrac{1}{2}q_0 + q_1)e^{g(x)/2} \equiv \psi_1(x). \quad (\text{A.4})$$

The characteristics of equation (A.2) are the straight lines $x \pm t = \text{const.}$ According to the Riemann method [32] if the characteristics go through the point M and intersect with the curve Γ at the points P and Q , then the solution of equation (A.2) at the point M can be represented as

$$\begin{aligned} u(M) &= \frac{1}{2}(u_P + u_Q) - \\ &- \frac{1}{2} \int_{PQ} v \left(\frac{\partial u}{\partial x_1} dt_1 + \frac{\partial u}{\partial t_1} dx_1 \right) - u \left(\frac{\partial v}{\partial x_1} dt_1 + \frac{\partial v}{\partial t_1} dx_1 \right) \end{aligned} \quad (\text{A.5})$$

The integral in (A.5) is taken along the curve Γ from P up Q and u_P and u_Q are the values of u , taken at the points P and Q . The Riemann function $v(M, M_1)$ for equation (A.3) has the form

$$v(M, M_1) = J_0 \left(\frac{1}{2} \sqrt{(x - x_1)^2 - (t - t_1)^2} \right), \quad (\text{A.6})$$

where $J_0(x)$ is the Bessel function of zero order and $\partial u / \partial x$ is calculated along the curve as

$$\left. \frac{\partial u}{\partial x} \right|_{t=g(x)} = \varphi_1'(x) - \psi_1(x)g'(x). \quad (\text{A.7})$$

The Riemann method for arbitrary linear hyperbolic equations can be found, for example, in [32].

Now consider the solution of equation (A.3) in the region $x \geq 0$, $t \leq 0$, $X = x + \alpha t < 0$, when the initial data are given at the straight line $t = -x/\alpha$ (see Figure A.1b). Instead of (A.3) and (A.4) we have

$$u|_{t=-x/\alpha} = q_0(x)e^{-x/2\alpha} \quad (\text{A.8})$$

$$\left. \frac{\partial u}{\partial t} \right|_{t=-x/\alpha} = \left(\frac{1}{2}q_0 + q_1 \right) e^{-x/2\alpha}. \quad (\text{A.9})$$

If the point M has coordinates (x, t) , so it is easy to show that the points P and Q have the abscissas respectively equal to

$$x_P = -\frac{\alpha(x+t)}{1-\alpha}; \quad x_Q = \frac{\alpha(x-t)}{1+\alpha} \quad (\text{A.10})$$

Consider the integral term in equation (A.5). Using equations (A.7)-(A.10) and the fact that along the pathway of integration $dt_1 = -dx_1/\alpha$, one has

$$\frac{1}{2} \int_{-\frac{\alpha(x+t)}{1-\alpha}}^{\frac{\alpha(x-t)}{1+\alpha}} dx_1 e^{-x_1/2\alpha} \left\{ v\psi(x_1) + \varphi(x_1) \left(\frac{1}{\alpha} \frac{\partial v}{\partial x_1} - \frac{\partial v}{\partial t_1} \right) \right\}_{t_1=-x_1/\alpha}, \quad (\text{A.11})$$

where the notations are introduced

$$\begin{aligned} \varphi(x) &= q_0(x), \\ \psi(x) &= \frac{1}{2}q_0(x) - \frac{1}{\alpha}q'_0(x) - \frac{1-\alpha^2}{\alpha^2}q_1(x). \end{aligned}$$

Furthermore using the Riemann function (A.6), it can show that

$$\left(\frac{1}{\alpha} \frac{\partial v}{\partial x_1} - \frac{\partial v}{\partial t_1} \right) \Big|_{t_1=-x_1/\alpha} = -\frac{X}{2\alpha} \frac{J'_0 \left(\frac{1}{2} \sqrt{(x-x_1)^2 - (t+x_1/\alpha)^2} \right)}{\sqrt{(x-x_1)^2 - (t+x_1/\alpha)^2}}. \quad (\text{A.12})$$

Finally, after substitution of integral (A.11) into equation (A.5) and using the equality $\tilde{q} = e^{-t/2}u$, one obtains the solution of the starting equation (A.1), with added conditions (14), in the form represented by (15).

Appendix B. The calculation of the integrals

Substituting equations (17) and (18) into (15) we have

$$\tilde{q}_L(x, t) = \sum_{n \geq 0} \tilde{J}_n(x, t), \quad (\text{B.1})$$

where

$$\begin{aligned} \tilde{J}_n(x, t) &= -B_n J_n^{(1)} + A_n J_n^{(2)} + \\ &+ \frac{A_n}{2} \left\{ \exp \left[\frac{\alpha \gamma_n (x+t) + X}{2(1-\alpha)} \right] + \exp \left[-\frac{\alpha \gamma_n (x-t) + X}{2(1+\alpha)} \right] \right\} \end{aligned} \quad (\text{B.2})$$

and

$$J_n^{(1)} = \frac{1}{2} e^{-t/2} \int_{-\frac{\alpha(x+t)}{1-\alpha}}^{\frac{\alpha(x-t)}{1+\alpha}} dx_1 e^{-x_1/2\delta_n} J_0\left(\frac{1}{2}\sqrt{(x-x_1)^2 - (t+x_1/\alpha)^2}\right); \quad (\text{B.3})$$

$$J_n^{(2)} = \frac{X}{4\alpha} e^{-t/2} \int_{-\frac{\alpha(x+t)}{1-\alpha}}^{\frac{\alpha(x-t)}{1+\alpha}} dx_1 e^{-x_1/2\delta_n} \frac{J'_0\left(\frac{1}{2}\sqrt{(x-x_1)^2 - (t+x_1/\alpha)^2}\right)}{\sqrt{(x-x_1)^2 - (t+x_1/\alpha)^2}}; \quad (\text{B.4})$$

$$\delta_n = \frac{\alpha}{1 + \alpha\gamma_n}. \quad (\text{B.5})$$

The calculation of $J_n^{(1)}$

Making the substitution in the integral (B.3)

$$\frac{2\alpha X}{1-\alpha^2} z = \frac{\alpha(x+t)}{1-\alpha} + x_1,$$

we have (for convenience the index n is omitted)

$$J^{(1)} = \frac{\alpha X}{1-\alpha^2} \exp\left[\frac{X'}{2(1-\alpha)}\right] \mathcal{J}, \quad (\text{B.6})$$

where the following notations are introduced

$$\mathcal{J} = \int_0^1 e^{-\mu z} J_0\left(\beta\sqrt{z(1-z)}\right) dz, \quad (\text{B.7})$$

$$X' = X + \left(\frac{\alpha}{\delta} - 1\right)(x+t), \quad (\text{B.8})$$

$$\mu = \frac{\alpha X}{\delta(1-\alpha^2)} < 0, \quad \beta = -\frac{X}{\sqrt{1-\alpha^2}} > 0. \quad (\text{B.9})$$

Consider the integral \mathcal{J} . Using the definition of the Bessel function

$$J_0\left(\beta\sqrt{z-z^2}\right) = \sum_{m=0}^{\infty} \frac{(-1)^m (\beta/2)^{2m} (z-z^2)^m}{m! \Gamma(m+1)},$$

where $\Gamma(x)$ is the Euler gamma-function, one represents the integral (B.7) in the form

$$\mathcal{J} = \sum_{m=0}^{\infty} \frac{(-1)^m (\beta/2)^{2m}}{m! \Gamma(m+1)} \int_0^1 e^{-\mu z} (z - z^2)^m dz \quad (\text{B.10})$$

Calculating the latter integral [33], one obtains

$$\mathcal{J} = \left(\pi/|\mu| \right)^{1/2} e^{-\mu} \sum_{n=0}^{\infty} \frac{(-\beta^2/4|\mu|)^n}{n!} I_{n+1/2} \left(\frac{|\mu|}{2} \right), \quad (\text{B.11})$$

where $I_\nu(x)$ is the modified Bessel function of the first kind. Furthermore, we use the equality [34]

$$\sum_{m=0}^{\infty} \frac{t^m}{m!} I_{m+1/2}(z) = \left(\frac{2t}{z} + 1 \right)^{-1/4} I_{1/2} \left(\sqrt{z^2 + 2tz} \right) \\ |z| - |2t| > 0. \quad (\text{B.12})$$

In our case

$$|z| - |2t| = \frac{\delta|X|}{2\alpha(1-\alpha^2)} (\alpha^2\gamma^2 + 2\alpha\gamma + \alpha^2) > 0$$

and instead of equation (B.11) we have

$$\mathcal{J} = \sqrt{\frac{\pi}{\nu|\mu|}} e^{-\mu/2} I_{1/2} \left(\frac{\nu|\mu|}{2} \right), \quad (\text{B.13})$$

where

$$\nu = \nu(\delta) = \sqrt{1 - \frac{\delta^2}{\alpha^2}(1 - \alpha^2)} = \frac{\delta}{\alpha} \sqrt{\alpha^2\gamma^2 + 2\alpha\gamma + \alpha^2}. \quad (\text{B.14})$$

Substituting the expression (B.13) into equation (B.6) and taking into account that $I_{1/2}(x) = (2/\pi x)^{1/2} \sinh(x)$, we obtain

$$J_n^{(1)} = \frac{\delta_n}{\nu_n} \exp \left[\frac{X'}{2(1-\alpha)} \right] \times \\ \times \left\{ \exp \left[-\frac{\alpha(1-\nu_n)X}{2\delta_n(1-\alpha^2)} \right] - \exp \left[-\frac{\alpha(1+\nu_n)X}{2\delta_n(1-\alpha^2)} \right] \right\}, \quad (\text{B.15})$$

where $\nu_n = \nu(\delta_n)$. At last, substituting X' from Eq. (B.8) into Eq. (B.15) one has

$$J_n^{(1)} = \frac{\delta_n}{\nu_n} e^{-\gamma_n x/2} \left\{ \exp \left[\frac{\gamma_n^{(+)} X}{2(1-\alpha^2)} \right] - \exp \left[\frac{\gamma_n^{(-)} X}{2(1-\alpha^2)} \right] \right\} \quad (\text{B.16})$$

and

$$\gamma_n^{(\pm)} = \alpha + \gamma_n \pm \sqrt{\alpha^2 \gamma_n^2 + 2\alpha \gamma_n + \alpha^2}.$$

The calculation of $J_n^{(2)}$

Consider the integral $J_n^{(2)}$. After substitution of the variable in equation (B.4)

$$\xi + \frac{X}{1-\alpha^2} = x - x_1 \quad (\text{B.17})$$

we have (the index n is omitted)

$$\begin{aligned} J^{(2)} &= -\frac{X}{4\alpha} \exp \left[\frac{X'}{2(1-\alpha)} - \frac{\alpha X}{2\delta(1-\alpha^2)} \right] \times \\ &\times \int_{\frac{\alpha X}{1-\alpha^2}}^{-\frac{\alpha X}{1-\alpha^2}} d\xi e^{\xi/2\delta} \frac{J'_0 \left(\frac{1}{2} \sqrt{\frac{1-\alpha^2}{\alpha^2}} \sqrt{\left(\frac{\alpha X}{1-\alpha^2} \right)^2 - \xi^2} \right)}{\sqrt{\frac{1-\alpha^2}{\alpha^2}} \sqrt{\left(\frac{\alpha X}{1-\alpha^2} \right)^2 - \xi^2}}. \quad (\text{B.18}) \end{aligned}$$

To calculate the integral (B.18) we consider the equality (B.15), having previously made the substitution (B.17) into $J_n^{(1)}$. After reducing common factors, we have

$$\begin{aligned} &\int_{\frac{\alpha X}{1-\alpha^2}}^{-\frac{\alpha X}{1-\alpha^2}} d\xi e^{\xi/2\delta} J_0 \left(\frac{1}{2} \sqrt{\frac{1-\alpha^2}{\alpha^2}} \sqrt{\left(\frac{\alpha X}{1-\alpha^2} \right)^2 - \xi^2} \right) = \\ &= -\frac{4\delta}{\nu} \sinh \left[\frac{\alpha \nu X}{2\delta(1-\alpha^2)} \right]. \quad (\text{B.19}) \end{aligned}$$

Differentiating the latter equation with respect to X , one obtains

$$\begin{aligned} \frac{X}{4\alpha} \int_{\frac{\alpha X}{1-\alpha^2}}^{-\frac{\alpha X}{1-\alpha^2}} d\xi e^{\xi/2\delta} \frac{J'_0\left(\frac{1}{2}\sqrt{\frac{1-\alpha^2}{\alpha^2}}\sqrt{\left(\frac{\alpha X}{1-\alpha^2}\right)^2 - \xi^2}\right)}{\sqrt{\frac{1-\alpha^2}{\alpha^2}}\sqrt{\left(\frac{\alpha X}{1-\alpha^2}\right)^2 - \xi^2}} = \\ = \cosh \frac{\alpha X}{2\delta(1-\alpha^2)} - \cosh \frac{\alpha\nu X}{2\delta(1-\alpha^2)}. \end{aligned} \quad (\text{B.20})$$

One multiplies the latter equality by

$$-\exp\left[\frac{X'}{2(1-\alpha)} - \frac{\alpha X}{2\delta(1-\alpha^2)}\right]$$

and using equations (B.18), (B.5) and (B.8), one has

$$\begin{aligned} J_n^{(2)} = \frac{1}{2} e^{-\gamma_n x/2} \left\{ \exp \frac{\gamma_n^{(+)} X}{2(1-\alpha^2)} + \exp \frac{\gamma_n^{(-)} X}{2(1-\alpha^2)} \right\} - \\ - \frac{1}{2} \left\{ \exp \left[\frac{\alpha\gamma_n(x+t) + X}{2(1-\alpha)} \right] + \exp \left[-\frac{\alpha\gamma_n(x-t) + X}{2(1+\alpha)} \right] \right\}. \end{aligned} \quad (\text{B.21})$$

Finally, substitute equations (B.16) and (B.21) into equation (B.2) and as a result we have

$$\tilde{J}_n(xt) = e^{-\gamma_n x/2} \left\{ A_n^{(-)} \exp \left[\frac{\gamma_n^{(+)} X}{2(1-\alpha^2)} \right] + A_n^{(+)} \exp \left[\frac{\gamma_n^{(-)} X}{2(1-\alpha^2)} \right] \right\}, \quad (\text{B.22})$$

where

$$A_n^{(\pm)} = \frac{A_n}{2} \pm B_n \frac{\delta_n}{\nu_n}.$$

Appendix C. The determination of the parameters of the equations (33)-(36)

For the determination parameters entering (33)-(36) we use the condition continuity of the temperature across the interface, $\tilde{T}_L = \tilde{T}_S$, and the condition of the heat balance (12). For this purpose initially we write down the latent heat of solidification $Q = kT_i$, with $T_i = T_L|_{X=0} = T_S|_{X=0}$, in dimensionless form as

$$\tilde{Q} = Q/Q_m = 1 + b\tilde{T}_S|_{X=0}, \quad (\text{C.1})$$

where $b = Q_m / \rho c_p T_m$.

Now we equate the temperatures \tilde{T}_S and \tilde{T}_L at the interface and substitute the fluxes (34), (36) at $X = 0$ into the condition of the heat balance (12), then taking into account the equalities (26), one obtains

$$ba_0^{(S)} + A_0/\alpha = -1 \quad (\text{C.2})$$

$$a_0^{(S)} + A_0/\alpha = \Delta \quad (\text{C.3})$$

$$A_n^{(S)} = \frac{nA_n}{n-b} \quad (n \geq 1) \quad (\text{C.4})$$

$$\frac{A_{n+1}^{(+)}}{n+1} + \frac{A_n^{(+)}}{n} = \frac{A_n}{n-b} \quad (n \geq 1) \quad (\text{C.5})$$

From the last equation of (26) and the equality (21) it follows that

$$A_n^{(+)} - A_{n+1}^{(+)} = A_n. \quad (\text{C.6})$$

The substitution of this equality into (C.5) gives the recurrent relationship

$$A_{n+1}^{(+)} = \frac{b(n+1)}{n(2n+1-b)} A_n^{(+)} \quad (n \geq 1),$$

whence one obtains

$$A_n^{(+)} = -\frac{nb^{n-1}}{(3-b)(5-b)\dots(2n-1-b)} A_0 \quad (n \geq 2), \quad (\text{C.7})$$

where the equality $A_1^{(+)} = -A_0$ has been used (see the relationships (26)). The remaining parameters A_0 and $a_0^{(S)}$ are found from the solution of the system (C.2) and (C.3) in the form

$$A_0 = -\alpha \frac{1+b\Delta}{1-b}, \quad a_0^{(S)} = \frac{1+\Delta}{1-b}. \quad (\text{C.8})$$

Finally, taking into account the equalities (C.4), (C.7) and (C.8), the expressions for the temperature of both the liquid and solid phase can be presented in the dimensional coordinates (x, t) in the form of the equations (37) and (38).

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Abstract

Keywords:

1.